Structural dynamics of nanoalloy catalysts for Fuel Cells by *in situ t*otal x-ray scattering

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Many catalysts for energy related applications, in particular metallic nanoalloys, readily undergo atomic-level changes during the electrochemical reactions driving the applications. The origin, dynamics and impact of the changes on the performance of the catalysts under actual operating conditions are, however, not well understood. This is largely because they are studied on model nanocatalysts under controlled laboratory conditions. We will present results from recent studies [1, 2, 3] on the dynamic behavior of metallic nanoalloy catalysts inside an operating proton exchange membrane fuel cell. Results show that their atomic structure changes profoundly, from the initial state to the active form and further along the cell operation. The electrocatalytic activity of the nanoalloys also changes. The rate and magnitude of the changes may be rationalized when the limits of traditional relationships used to connect the composition and structure of nanoalloys with their electrocatalytic activity and stability, such as Vegard's law, are recognized. In particular, deviations from the law can well explain the behaviour for Pt-3d metal nanoalloy catalysts under operating conditions. Moreover, it appears that factors behind their remarkable electrocatalytic activity, such as the large surface to volume ratio and "misfit" between the size of constituent atoms, are indeed detrimental to their stability inside fuel cells. The new insight into the atomic-level evolution of nanoalloy electrocatalysts during their usage is likely to inspire new efforts to stabilize transient structure states beneficial to their activity and stability under operating conditions, if not synthesize them directly.

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2. Zh. Kong et al. J. Am. Chem. Soc. 142, 1287 (2020).

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